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Appl. No. 10/791,681; Filed: Mar 3, 2004
Dkt No. 1866.0220001/PEG/CMB; Group Unit: 2857
Inventor: Frank P. HOLLINGER, Ph.D. Tel: 202-371-2600
Title: Methods and Systems for Preparing Virtual Representations of Molecules

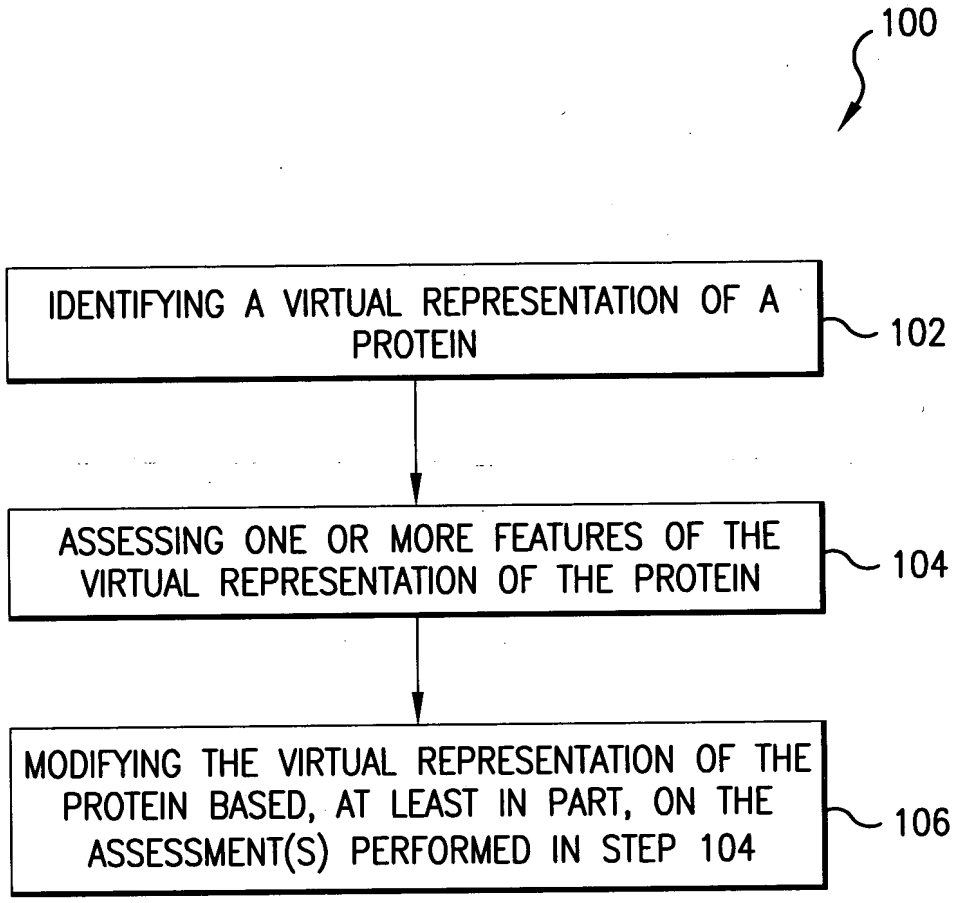

FIG. 1

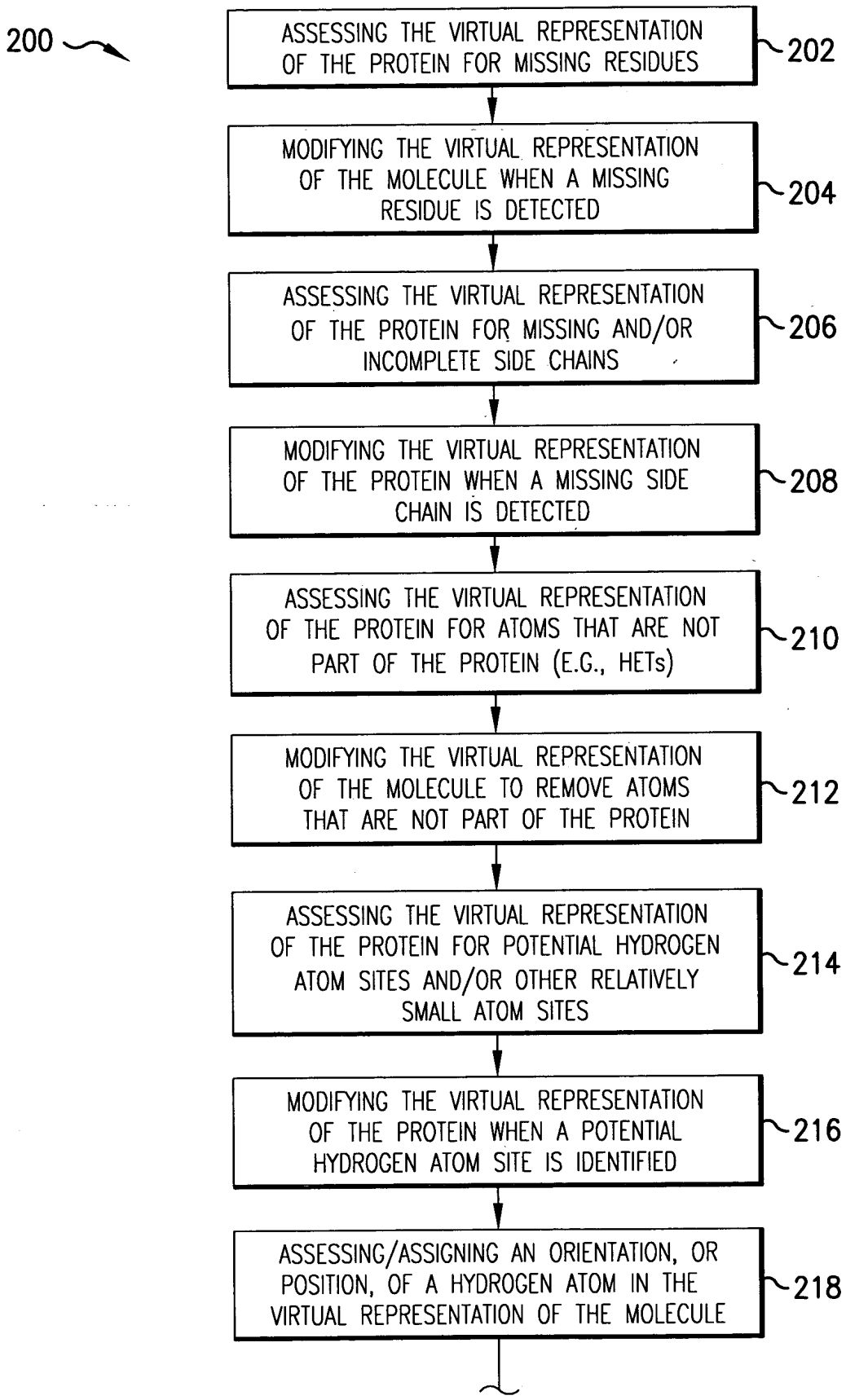
200
ASSESSING THE VIRTUAL REPRESENTATION OF THE PROTEIN FOR MISSING RESIDUES
202
MODIFYING THE VIRTUAL REPRESENTATION OF THE MOLECULE WHEN A MISSING RESIDUE IS DETECTED
204
ASSESSING THE VIRTUAL REPRESENTATION OF THE PROTEIN FOR MISSING AND/OR INCOMPLETE SIDE CHAINS
206
MODIFYING THE VIRTUAL REPRESENTATION OF THE PROTEIN WHEN A MISSING SIDE CHAIN IS DETECTED
208
ASSESSING THE VIRTUAL REPRESENTATION OF THE PROTEIN FOR ATOMS THAT ARE NOT PART OF THE PROTEIN (E.G., HETs)
210
MODIFYING THE VIRTUAL REPRESENTATION OF THE MOLECULE TO REMOVE ATOMS THAT ARE NOT PART OF THE PROTEIN
212
ASSESSING THE VIRTUAL REPRESENTATION OF THE PROTEIN FOR POTENTIAL HYDROGEN ATOM SITES AND/OR OTHER RELATIVELY SMALL ATOM SITES
214
MODIFYING THE VIRTUAL REPRESENTATION OF THE PROTEIN WHEN A POTENTIAL HYDROGEN ATOM SITE IS IDENTIFIED
216
ASSESSING/ASSIGNING AN ORIENTATION, OR POSITION, OF A HYDROGEN ATOM IN THE VIRTUAL REPRESENTATION OF THE MOLECULE
218

FIG.2A

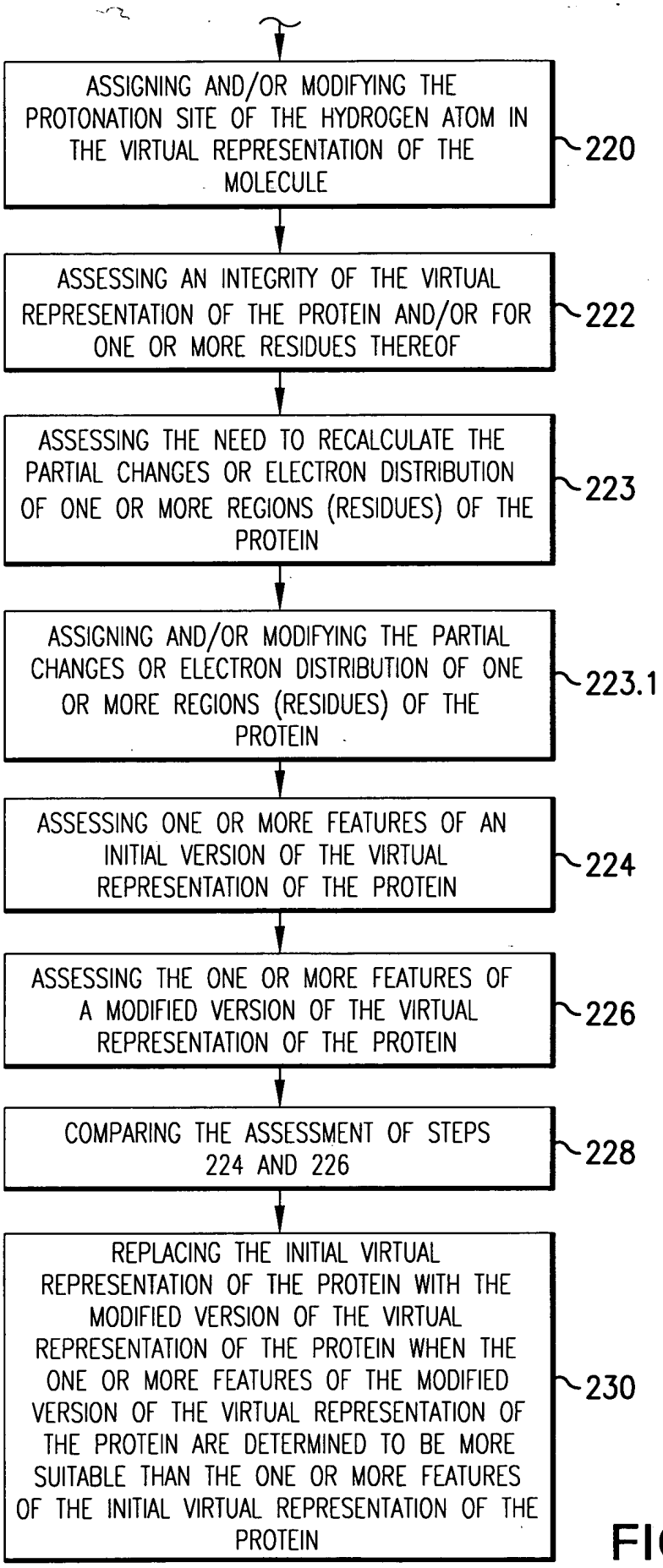
ASSIGNING AND/OR MODIFYING THE PROTONATION SITE OF THE HYDROGEN ATOM IN THE VIRTUAL REPRESENTATION OF THE MOLECULE
220
ASSESSING AN INTEGRITY OF THE VIRTUAL REPRESENTATION OF THE PROTEIN AND/OR FOR ONE OR MORE RESIDUES THEREOF
222
ASSESSING THE NEED TO RECALCULATE THE PARTIAL CHANGES OR ELECTRON DISTRIBUTION OF ONE OR MORE REGIONS (RESIDUES) OF THE PROTEIN
223
ASSIGNING AND/OR MODIFYING THE PARTIAL CHANGES OR ELECTRON DISTRIBUTION OF ONE OR MORE REGIONS (RESIDUES) OF THE PROTEIN
223.1
ASSESSING ONE OR MORE FEATURES OF AN INITIAL VERSION OF THE VIRTUAL REPRESENTATION OF THE PROTEIN
224
ASSESSING THE ONE OR MORE FEATURES OF A MODIFIED VERSION OF THE VIRTUAL REPRESENTATION OF THE PROTEIN
226
COMPARING THE ASSESSMENT OF STEPS 224 AND 226
228
REPLACING THE INITIAL VIRTUAL REPRESENTATION OF THE PROTEIN WITH THE MODIFIED VERSION OF THE VIRTUAL REPRESENTATION OF THE PROTEIN WHEN THE ONE OR MORE FEATURES OF THE MODIFIED VERSION OF THE VIRTUAL REPRESENTATION OF THE PROTEIN ARE DETERMINED TO BE MORE SUITABLE THAN THE ONE OR MORE FEATURES OF THE INITIAL VIRTUAL REPRESENTATION OF THE PROTEIN
230

FIG.2B

PDB
PROTEIN DATA BANK

Structure Explorer – 1AIK

Title Hiv Gp41 Core Structure

Classification Glycoprotein

Compound Mol_Id: 1; Molecule: Hiv-1 Gp41 Glycoprotein; Chain: N, C; Fragment: Protease-Resistant Core; Biological_Unit: Trimer; Other_Details: N36 and C34 Are Synthetic Peptides

Exp. Method X-ray Diffraction

Download/Display File

Summary Information

View Structure

Download/Display File

Structural Neighbors

Geometry

Other Sources

Sequence Details

SearchLite SearchFields

Save full entry to disk

```
HEADER    GLYCOPROTEIN                                20-APR-97   1AIK
TITLE     HIV GP41 CORE STRUCTURE
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: HIV-1 GP41 GLYCOPROTEIN;
COMPND   3 CHAIN: N, C;
COMPND   4 FRAGMENT: PROTEASE-RESISTANT CORE;
COMPND   5 BIOLOGICAL_UNIT: TRIMER;
COMPND   6 OTHER_DETAILS: N36 AND C34 ARE SYNTHETIC PEPTIDES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1;
SOURCE   3 STRAIN: HXB2;
SOURCE   4 CELLULAR_LOCATION: VIRAL MEMBRANE
KEYWDS    HIV, GP41, ENVELOPE GLYCOPROTEIN, RETROVIRUS
EXPDTA    X-RAY DIFFRACTION
AUTHOR    D.C.CHAN, D. FASS, J.M. BERGER, P.S. KIM
REVDAT   1   16-JUN-97   1AIK      0
REMARK    1
```

FIG.3A

Sheet 4 of 22
Appl. No. 10/791,681; Filed: Mar 3, 2004
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```
REMARK   1  REFERENCE 1
REMARK   1    AUTH     D.C.CHAN,D.FASS,J.M.BERGER,P.S.KIM
REMARK   1    TITL     CORE STRUCTURE OF GP41 FROM THE HIV ENVELOPE
REMARK   1    TITL 2   GLYCOPROTEIN
REMARK   1    REF      CELL (CAMBRIDGE,MASS.)     V.  89   263 1997
REMARK   1    REFN     ASTM CELLB5   US ISSN 0092-8674           0998
REMARK   2
REMARK   2  RESOLUTION.    2.0  ANGSTROMS.
REMARK   3
REMARK   3  REFINEMENT.
REMARK   3    PROGRAM        : X-PLOR    3.851
REMARK   3    AUTHORS        : BRUNGER
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3     RESOLUTION RANGE HIGH (ANGSTROMS)  :  2.0
REMARK   3     RESOLUTION RANGE LOW  (ANGSTROMS)  :  12.0
REMARK   3     DATA CUTOFF            (SIGMA(F))  :  2.0
REMARK   3     DATA CUTOFF HIGH        (ABS (F))  :  100000000.
REMARK   3     DATA CUTOFF LOW         (ABS (F))  :  NULL
REMARK   3     COMPLETENESS (WORKING+TEST) (%)    :  96.5
REMARK   3     NUMBER OF REFLECTIONS              :  5683
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3     CROSS-VALIDATION METHOD            :  THROUGHOUT
REMARK   3     FREE R VALUE TEST SET SELECTION    :  RANDOM
REMARK   3     R VALUE            (WORKING SET)   :  0.238
REMARK   3     FREE R VALUE                       :  0.266
REMARK   3     FREE R VALUE TEST SET SIZE   (%)   :  7.12
REMARK   3     FREE R VALUE TEST SET COUNT        :  371
REMARK   3     ESTIMATED ERROR OF FREE R VALUE    :  NULL
REMARK   3
```

FIG.3B

Sheet 5 of 22
Appl. No. 10/791,681; Filed: Mar 3, 2004
Dkt No. 1866.022001/PEG/CMB; Group Unit: 2857
Inventor: Frank P. HOLLINGER, Ph.D. Tel: 202-371-260(
Title: Methods and Systems for Preparing Virtual
Representations of Molecules

```
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3    TOTAL NUMBER OF BINS USED           :  NULL
REMARK   3    BIN RESOLUTION RANGE HIGH      (A)  :  NULL
REMARK   3    BIN RESOLUTION RANGE LOW       (A)  :  NULL
REMARK   3    BIN COMPLETENESS (WORKING+TEST)(%)  :  NULL
REMARK   3    REFLECTIONS IN BIN   (WORKING SET)  :  NULL
REMARK   3    BIN R VALUE          (WORKING SET)  :  NULL
REMARK   3    BIN FREE R VALUE                    :  NULL
REMARK   3    BIN FREE R VALUE TEST SET SIZE (%)  :  NULL
REMARK   3    BIN FREE R VALUE TEST SET COUNT     :  NULL
REMARK   3    ESTIMATED ERROR OF BIN FREE R VALUE :  NULL
REMARK   3
REMARK   3   NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3      PROTEIN ATOMS          :  596
REMARK   3      NUCLEIC ACID ATOMS     :  0
REMARK   3      HETEROGEN ATOMS        :  0
REMARK   3      SOLVANT ATOMS          :  43
REMARK   3
REMARK   3   B VALUES.
REMARK   3      FROM WILSON PLOT           (A**2)    :  NULL
REMARK   3      MEAN B VALUE      (OVERALL, A**2)    :  NULL
REMARK   3      OVERALL ANISOTROPIC B VALUE.
REMARK   3         B11   (A**2)     :  NULL
REMARK   3         B22   (A**2)     :  NULL
REMARK   3         B33   (A**2)     :  NULL
REMARK   3         B12   (A**2)     :  NULL
REMARK   3         B13   (A**2)     :  NULL
REMARK   3         B23   (A**2)     :  NULL
REMARK   3
REMARK   3   ESTIMATED COORDINATE ERROR.
```

FIG.3C

```
REMARK   3      ESD FROM LUZZATI PLOT       (A)    :  NULL
REMARK   3      ESD FROM SIGMAA             (A)    :  NULL
REMARK   3      LOW RESOLUTION CUTOFF       (A)    :  NULL
REMARK   3
REMARK   3    CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3      ESD FROM C-V LUZZATI PLOT   (A)    :  NULL
REMARK   3      ESD FROM C-V SIGMAA         (A)    :  NULL
REMARK   3
REMARK   3    RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3      BOND LENGTHS                (A)    :  0.014
REMARK   3      BOND ANGLES           (DEGREES)    :  2.742
REMARK   3      DIHEDRAL ANGLES       (DEGREES)    :  NULL
REMARK   3      IMPROPER ANGLES       (DEGREES)    :  NULL
REMARK   3
REMARK   3    ISOTROPIC THERMAL MODEL : NULL
REMARK   3
REMARK   3    ISOTROPIC THERMAL FACTOR RESTRAINTS.      RMS          SIGMA
REMARK   3    MAIN-CHAIN BOND             (A**2)    :  NULL     ;   NULL
REMARK   3    MAIN-CHAIN ANGLE            (A**2)    :  NULL     ;   NULL
REMARK   3    SIDE-CHAIN BOND             (A**2)    :  NULL     ;   NULL
REMARK   3    SIDE-CHAIN ANGLE            (A**2)    :  NULL     ;   NULL
REMARK   3
REMARK   3   NCS MODEL  :  NULL
REMARK   3
REMARK   3   NCS RESTRAINTS.                          RMS          SIGMA/WEIGHT
REMARK   3    GROUP  1     POSITIONAL        (A)    :  NULL     ;   NULL
REMARK   3    GROUP  1     B-FACTOR        (A**2)   :  NULL     ;   NULL
REMARK   3
REMARK   3   PARAMETER FILE    1     :  NULL
REMARK   3   PARAMETER FILE    2     :  NULL
```

FIG.3D

Sheet 7 of 22
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Dkt No. 1866.022001/PEG/CMB; Group Unit: 2857
Inventor: Frank P. HOLLINGER, Ph.D. Tel: 202-371-2600
Title: Methods and Systems for Preparing Virtual Representations of Molecules

```
REMARK   3  TOPOLOGY FILE   1      :  NULL
REMARK   3  TOPOLOGY FILE   2      :  NULL
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS :  NULL
REMARK   4
REMARK   4  1AIK COMPILES WITH FORMAT V.  2.2,   16-DEC-1996
REMARK   6
REMARK   6  C-TERMINAL NH2 NOT IN ATOM LIST FOR BOTH CHAINS.
REMARK 200
REMARK 200  EXPERIMENTAL DETAILS
REMARK 200    EXPERIMENT TYPE                          :  X-RAY DIFFRACTION
REMARK 200    DATE OF DATA COLLECTION                  :  MAR-1997
REMARK 200    TEMPERATURE                (KELVIN)      :  100
REMARK 200    PH                                       :  6.0
REMARK 200    NUMBER OF CRYSTALS USED                  :  1
REMARK 200
REMARK 200    SYNCHROTRON                (Y/N)         :  N
REMARK 200    RADIATION SOURCE                         :  NULL
REMARK 200    BEAMLINE                                 :  NULL
REMARK 200    X-RAY GENERATOR MODEL                    :  RIGAKU RU200
REMARK 200   MONOCHROMATIC OR LAUE       (M/L)         :  M
REMARK 200   WAVELENGTH OR RANGE           (A)         :  1.5418
REMARK 200   MONOCHROMATOR                             :  NULL
REMARK 200   OPTICS                                    :  MIRRORS
REMARK 200
REMARK 200   DETECTOR TYPE                             :  R-AXIS IIC
REMARK 200   DETECTOR MANUFACTURER                     :  RIGAKU
REMARK 200   INTENSITY-INTEGRATION SOFTWARE            :  DENZO
REMARK 200   DATA SCALING SOFTWARE                     :  SCALEPACK
REMARK 200
REMARK 200   NUMBER OF UNIQUE REFLECTIONS              :  5287
REMARK 200   RESOLUTION RANGE HIGH      (A)           :  2.0
```

FIG.3E

Sheet 8 of 22
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```
REMARK 200   RESOLUTION RANGE LOW                (A)     :   20.0
REMARK 200   REJECTION CRITERIA          (SIGMA (I))     :   1.5
REMARK 200
REMARK 200 OVERALL.
REMARK 200   COMPLETENESS FOR RANGE              (%)     :   96.5
REMARK 200   DATA REDUNDANCY                             :   NULL
REMARK 200   R MERGE                             (I)     :   NULL
REMARK 200   R SYM                               (I)     :   0.054
REMARK 200   < I/SIGMA (I) > FOR THE DATA SET            :   18.4
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200   HIGHEST RESOLUTION SHELL, RANGE HIGH              (A)     :   2.00
REMARK 200   HIGHEST RESOLUTION SHELL, RANGE LOW               (A)     :   2.07
REMARK 200   COMPLETENESS FOR SHELL              (%)     :   98.9
REMARK 200   DATA REDUNDANCY IN SHELL                     :   NULL
REMARK 200   R MERGE FOR SHELL                  (I)     :   NULL
REMARK 200   R SYM FOR SHELL                    (I)     :   0.263
REMARK 200   < I/SIGMA (I) > FOR SHELL                   :   5.4
REMARK 200
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE:  MAD
REMARK 200 SOFTWARE USED:  CCP4 SUITE
REMARK 200 STARTING MODEL:  NULL
REMARK 200
REMARK 200 REMARK:  DATA AT NSLS USED MAD METHODS.  DATA COLLECTED ON
REMARK 200 AN OSMIUM-SOAK CRYSTAL AT WAVELENGTHS  1.1398, 1.1396,
REMARK 200 1.1344, AND 1.1406 ANGSTOMS.
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT,  VS       (%)  : 46.
REMARK 280 MATTHEWS COEFFICIENT, VM  (ANGSTROMS**3/DA)  :  NULL
REMARK 280
```

FIG.3F

Sheet 9 of 22
Appl. No. 10/791,681; Filed: Mar 3, 2004
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Title: Methods and Systems for Preparing Virtual Representations of Molecules

```
REMARK 280 CRYSTALLIZATION CONDITIONS:  A 10 MG/ML STOCK WAS DILUTED
REMARK 280 1:1 IN A SITTING DROP WITH 80 MM NH4CL, 20 % PEG200, AND
REMARK 280 50 % ISOPROPANOL, AND THEN ALLOWED TO EQUILIBRATE AGAINST
REMARK 280 80 MM NH4CL, 20 % PEG200, AND 30 % ISOPROPANOL.
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP:  P  3  2  1
REMARK 290
REMARK 290          SYMOP    SYMMETRY
REMARK 290         NNNMMM    OPERATOR
REMARK 290                   1555      X,Y,Z
REMARK 290                   2555      -Y,X-Y,Z
REMARK 290                   3555      Y-X,-X,Z
REMARK 290                   4555      Y,X,-Z
REMARK 290                   5555      X-Y,-Y,-Z
REMARK 290                   6555      -X,Y-X,-Z
REMARK 290
REMARK 290          WHERE NNN  -> OPERATOR NUMBER
REMARK 290                MMM  -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290      SMTRY1    1     1.000000    0.000000    0.000000    0.00000
REMARK 290      SMTRY2    1     0.000000    1.000000    0.000000    0.00000
REMARK 290      SMTRY3    1     0.000000    0.000000    1.000000    0.00000
REMARK 290      SMTRY1    2    -0.500021   -0.866016    0.000000    0.00000
REMARK 290      SMTRY2    2     0.866035   -0.499979    0.000000    0.00000
REMARK 290      SMTRY3    2     0.000000    0.000000    1.000000    0.00000
REMARK 290      SMTRY1    3    -0.499979    0.866016    0.000000    0.00000
REMARK 290      SMTRY2    3    -0.866035   -0.500021    0.000000    0.00000
```

FIG.3G

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```
REMARK 290      SMTRY3    3     0.000000    0.000000    1.000000    0.00000
REMARK 290      SMTRY1    4    -0.500021    0.865991    0.000000    0.00000
REMARK 290      SMTRY2    4     0.866035    0.500021    0.000000    0.00000
REMARK 290      SMTRY3    4     0.000000    0.000000   -1.000000    0.00000
REMARK 290      SMTRY1    5     1.000000    0.000050    0.000000    0.00000
REMARK 290      SMTRY2    5     0.000000   -1.000000    0.000000    0.00000
REMARK 290      SMTRY3    5     0.000000    0.000000   -1.000000    0.00000
REMARK 290      SMTRY1    6    -0.499979   -0.866041    0.000000    0.00000
REMARK 290      SMTRY2    6    -0.866035    0.499979    0.000000    0.00000
REMARK 290      SMTRY3    6     0.000000    0.000000   -1.000000    0.00000
REMARK 290
REMARK 290 REMARK:  NULL
REMARK 999
REMARK 999 SEQUENCE
REMARK 999 1AIK      C         SWS          P04582          1  -     621 NOT IN ATOMS LIST
REMARK 999 1AIK      C         SWS          P04582        657  -     851 NOT IN ATOMS LIST
REMARK 999 1AIK      N         SWS          P19551          1  -     542 NOT IN ATOMS LIST
REMARK 999 1AIK      N         SWS          P19551        580  -     853 NOT IN ATOMS LIST
DBREF  1AIK C          0       661     SWS      P04582     ENV_HV1B8     622          656
DBREF  1AIK N          0       581     SWS      P19551     ENV_HV1MF     543          579
SEQADV 1AIK ACE    C       0    SWS     P04582     THR        622  CONFLICT
SEQADV 1AIK ACE    N       0    SWS     P19551     LEU        543  CONFLICT
SEQRES   1  N         38   ACE SER GLY ILE VAL GLN GLN GLN ASN ASN LEU LEU ARG
SEQRES   2  N         38   ALA ILE GLU ALA GLN GLN HIS LEU LEU GLN LEU THR VAL
SEQRES   3  N         38   TRP GLY ILE LYS GLN LEU GLN ALA ARG ILE LEU NH2
SEQRES   1  C         36   ACE TRP MET GLU TRP ASP ARG GLU ILE ASN ASN TYR THR
SEQRES   2  C         36   SER LEU ILE HIS SER LEU ILE GLU GLU SER GLN ASN GLN
SEQRES   3  C         36   GLN GLU LYS ASN GLU GLN GLU LEU LEU NH2
HET    ACE     N       0        3
HET    ACE     C       0        3
HETNAM          ACE ACETYL GROUP
FORMUL   1       ACE         C2  H3  01
```

FIG.3H

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Title: Methods and Systems for Preparing Virtual Representations of Molecules

```
FORMUL   2       ACE          C2  H3  01
FORMUL   3       HOH          *43 (H2  01)
HELIX    1       1  GLY  N    547   ALA  N    578   1                                                  32
HELIX    2       2  MET  C    629   GLU  C    659   1                                                  31
LINK             C        ACE  N        0                          N     SER  N  546
LINK             C        ACE  C        0                          N     TRP  C  628
CRYST1     49.500     49.500      55.300    90.00     90.00    120.00    P 3 2 1    6
ORIGX1      1.000000              0.000000              0.000000                        0.00000
ORIGX2      0.000000              1.000000              0.000000                        0.00000
ORIGX3      0.000000              0.000000              1.000000                        0.00000
SCALE1      0.020202              0.011664              0.000000                        0.00000
SCALE2      0.000000              0.023327              0.000000                        0.00000
SCALE3      0.000000              0.000000              0.018083                        0.00000
HETATM   1   C    ACE  N    0     19.211   14.270   -17.472   1.00    56.26      C
HETATM   2   O    ACE  N    0     19.488   14.580   -16.305   1.00    56.37      O
HETATM   3   CH3  ACE  N    0     20.273   14.045   -18.531   1.00    56.01      C
ATOM     4   N    SER  N  546     17.955   14.014   -17.827   1.00    56.49      N
ATOM     5   CA   SER  N  546     16.876   14.392   -16.942   1.00    56.15      C
ATOM     6   C    SER  N  546     16.909   13.631   -15.655   1.00    56.24      C
ATOM     7   O    SER  N  546     16.736   14.255   -14.615   1.00    57.67      O
ATOM     8   CB   SER  N  546     15.525   14.172   -17.546   1.00    56.05      C
ATOM     9   OG   SER  N  546     15.498   12.815   -17.842   1.00    57.84      O
ATOM     10  H    SER  N  546     17.816   13.501   -18.652   1.00    0.00       H
ATOM     11  HG   SER  N  546     15.988   12.455   -18.582   1.00    0.00       H
ATOM     12  N    GLY  N  547     17.181   12.316   -15.724   1.00    55.59      N
ATOM     13  CA   GLY  N  547     17.202   11.414   -14.570   1.00    53.04      C
ATOM     14  C    GLY  N  547     18.299   11.783   -13.596   1.00    51.70      C
ATOM     15  O    GLY  N  547     18.147   11.667   -12.391   1.00    50.76      O
ATOM     16  H    GLY  N  547     17.409   11.945   -16.618   1.00    0.00       H
ATOM     17  N    ILE  N  548     19.399   12.280   -14.145   1.00    51.57      N
ATOM     18  CA   ILE  N  548     20.551   12.815   -13.425   1.00    52.14      C
```

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FIG.3I

302

ATOM	19	C	ILE	N	548	20.218	14.116	-12.696	1.00	51.31	C
ATOM	20	O	ILE	N	548	20.543	14.273	-11.519	1.00	50.83	O
ATOM	21	CB	ILE	N	548	21.693	13.043	-14.436	1.00	54.22	C
ATOM	22	CG1	ILE	N	548	22.120	11.712	-15.087	1.00	54.58	C
ATOM	23	CG2	ILE	N	548	22.861	13.705	-13.721	1.00	55.25	C
ATOM	24	CD1	ILE	N	548	23.126	11.909	-16.234	1.00	56.29	C
ATOM	25	H	ILE	N	548	19.445	12.272	-15.118	1.00	0.00	H
ATOM	26	N	VAL	N	549	19.590	15.054	-13.393	1.00	50.93	N
ATOM	27	CA	VAL	N	549	19.093	16.291	-12.786	1.00	50.79	C
ATOM	28	C	VAL	N	549	18.036	15.977	-11.726	1.00	50.36	C
ATOM	29	O	VAL	N	549	17.992	16.598	-10.674	1.00	51.60	O
ATOM	30	CB	VAL	N	549	18.451	17.196	-13.841	1.00	52.28	C
ATOM	31	CG1	VAL	N	549	17.814	18.437	-13.226	1.00	54.97	C
ATOM	32	CG2	VAL	N	549	19.539	17.650	-14.780	1.00	51.05	C
ATOM	33	H	VAL	N	549	19.486	14.911	-14.360	1.00	0.00	H
ATOM	34	N	GLN	N	550	17.187	15.030	-12.001	1.00	49.13	N
ATOM	35	CA	GLN	N	550	16.176	14.508	-11.109	1.00	49.23	C
ATOM	36	C	GLN	N	550	16.843	13.895	-9.861	1.00	48.50	C
ATOM	37	O	GLN	N	550	16.520	14.236	-8.736	1.00	47.94	O
ATOM	38	CB	GLN	N	550	15.452	13.398	-11.814	1.00	52.96	C

FIG.3J

304	306	308	310	312	314	316					
HETATM	1	C	ACE	N	0	19.211	14.270	-17.472	1.00	56.26	C
HETATM	2	O	ACE	N	0	19.488	14.580	-16.305	1.00	56.37	O
HETATM	3	CH3	ACE	N	0	20.273	14.045	-18.531	1.00	56.01	C
ATOM	4	N	SER	N	546	17.955	14.014	-17.827	1.00	56.49	N
ATOM	5	CA	SER	N	546	16.876	14.392	-16.942	1.00	56.15	C
ATOM	6	C	SER	N	546	16.909	13.631	-15.655	1.00	56.24	C
ATOM	7	O	SER	N	546	16.736	14.255	-14.615	1.00	57.67	O
ATOM	8	CB	SER	N	546	15.525	14.172	-17.546	1.00	56.05	C
ATOM	9	OG	SER	N	546	15.498	12.815	-17.842	1.00	57.84	O
ATOM	10	H	SER	N	546	17.816	13.501	-18.652	1.00	0.00	H
ATOM	11	HG	SER	N	546	15.988	12.455	-18.582	1.00	0.00	H
ATOM	12	N	GLY	N	547	17.181	12.316	-15.724	1.00	55.59	N
ATOM	13	CA	GLY	N	547	17.202	11.414	-14.570	1.00	53.04	C
ATOM	14	C	GLY	N	547	18.299	11.783	-13.596	1.00	51.70	C
ATOM	15	O	GLY	N	547	18.147	11.667	-12.391	1.00	50.76	O
ATOM	16	H	GLY	N	547	17.409	11.945	-16.618	1.00	0.00	H
ATOM	17	N	ILE	N	548	19.399	12.280	-14.145	1.00	51.57	N
ATOM	18	CA	ILE	N	548	20.551	12.815	-13.425	1.00	52.14	C
ATOM	19	C	ILE	N	548	20.218	14.116	-12.696	1.00	51.31	C
ATOM	20	O	ILE	N	548	20.543	14.273	-11.519	1.00	50.83	O
ATOM	21	CB	ILE	N	548	21.693	13.043	-14.436	1.00	54.22	C
ATOM	22	CG1	ILE	N	548	22.120	11.712	-15.087	1.00	54.58	C
ATOM	23	CG2	ILE	N	548	22.861	13.705	-13.721	1.00	55.25	C
ATOM	24	CD1	ILE	N	548	23.126	11.909	-16.234	1.00	56.29	C
ATOM	25	H	ILE	N	548	19.445	12.272	-15.118	1.00	0.00	H
ATOM	26	N	VAL	N	549	19.590	15.054	-13.393	1.00	50.93	N
ATOM	27	CA	VAL	N	549	19.093	16.291	-12.786	1.00	50.79	C
ATOM	28	C	VAL	N	549	18.036	15.977	-11.726	1.00	50.36	C

FIG.3K

ATOM	29	O	VAL	N	549	17.992	16.598	-10.674	1.00	51.60	O
ATOM	30	CB	VAL	N	549	18.451	17.196	-13.841	1.00	52.28	C
ATOM	31	CG1	VAL	N	549	17.814	18.437	-13.226	1.00	54.97	C
ATOM	32	CG2	VAL	N	549	19.539	17.650	-14.780	1.00	51.05	C
ATOM	33	H	VAL	N	549	19.486	14.911	-14.360	1.00	0.00	H
ATOM	34	N	GLN	N	550	17.187	15.030	-12.001	1.00	49.13	N
ATOM	35	CA	GLN	N	550	16.176	14.508	-11.109	1.00	49.23	C
ATOM	36	C	GLN	N	550	16.843	13.895	-9.861	1.00	48.50	C
ATOM	37	O	GLN	N	550	16.520	14.236	-8.736	1.00	47.94	O
ATOM	38	CB	GLN	N	550	15.452	13.398	-11.814	1.00	52.96	C

FIG.3L

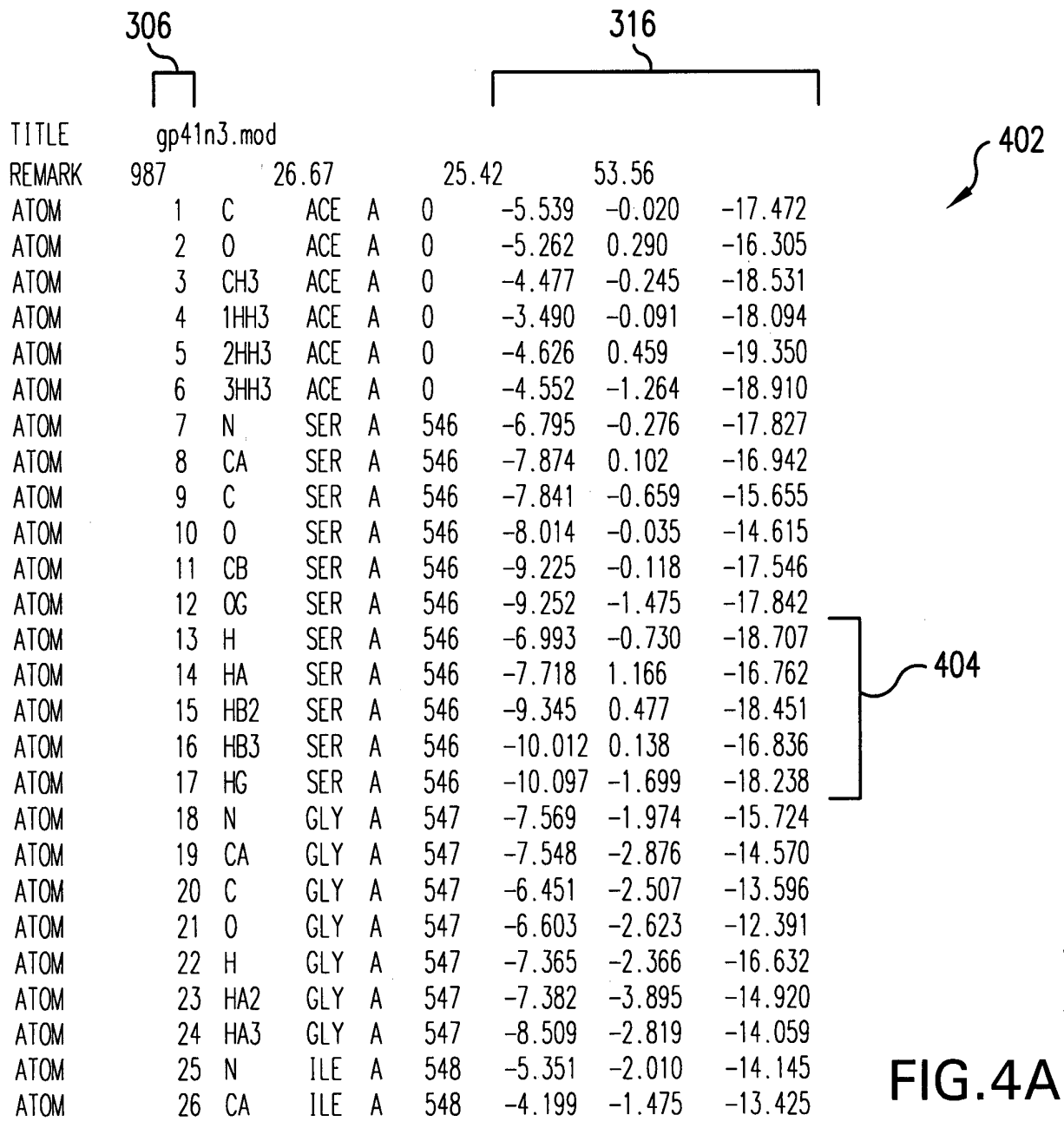


FIG.4A

Sheet 16 of 22
Appl. No. 10/791,681; Filed: Mar 3, 2004
Dkt No. 1866.022001/PEG/CMB; Group Unit: 2857
Inventor: Frank P. HOLLINGER, Ph.D. Tel: 202-371-2600
Title: Methods and Systems for Preparing Virtual Representations of Molecules

ATOM	27	C	ILE	A	548	-4.532	-0.174	-12.696
ATOM	28	O	ILE	A	548	-4.207	-0.017	-11.519
ATOM	29	CB	ILE	A	548	-3.057	-1.247	-14.436
ATOM	30	CG1	ILE	A	548	-2.630	-2.578	-15.087
ATOM	31	CG2	ILE	A	548	-1.889	-0.585	-13.721
ATOM	32	CD1	ILE	A	548	-1.624	-2.381	-16.234
ATOM	33	H	ILE	A	548	-5.306	-2.001	-15.154
ATOM	34	HA	ILE	A	548	-3.897	-2.193	-12.663
ATOM	35	HB	ILE	A	548	-3.403	-0.592	-15.236
ATOM	36	2HG1	ILE	A	548	-3.517	-3.073	-15.482
ATOM	37	3HG1	ILE	A	548	-2.171	-3.208	-14.325
ATOM	38	1HG2	ILE	A	548	-1.076	-0.420	-14.429
ATOM	39	2HG2	ILE	A	548	-1.543	-1.232	-12.915
ATOM	40	3HG2	ILE	A	548	-2.211	0.371	-13.307
ATOM	41	1HD1	ILE	A	548	-1.359	-3.351	-16.655
ATOM	42	2HD1	ILE	A	548	-0.727	-1.893	-15.851
ATOM	43	3HD1	ILE	A	548	-2.073	-1.759	-17.008
ATOM	44	N	VAL	A	549	-5.160	0.764	-13.393
ATOM	45	CA	VAL	A	549	-5.657	2.001	-12.786
ATOM	46	C	VAL	A	549	-6.714	1.687	-11.726
ATOM	47	O	VAL	A	549	-6.758	2.308	-10.674
ATOM	48	CB	VAL	A	549	-6.299	2.906	-13.841
ATOM	49	CG1	VAL	A	549	-6.936	4.147	-13.226
ATOM	50	CG2	VAL	A	549	-5.211	3.360	-14.780
ATOM	51	H	VAL	A	549	-5.301	0.619	-14.382
ATOM	52	HA	VAL	A	549	-4.805	2.508	-12.333
ATOM	53	HB	VAL	A	549	-7.080	2.340	-14.348
ATOM	54	1HG1	VAL	A	549	-7.378	4.757	-14.014
ATOM	55	2HG1	VAL	A	549	-6.174	4.725	-12.703

FIG.4B

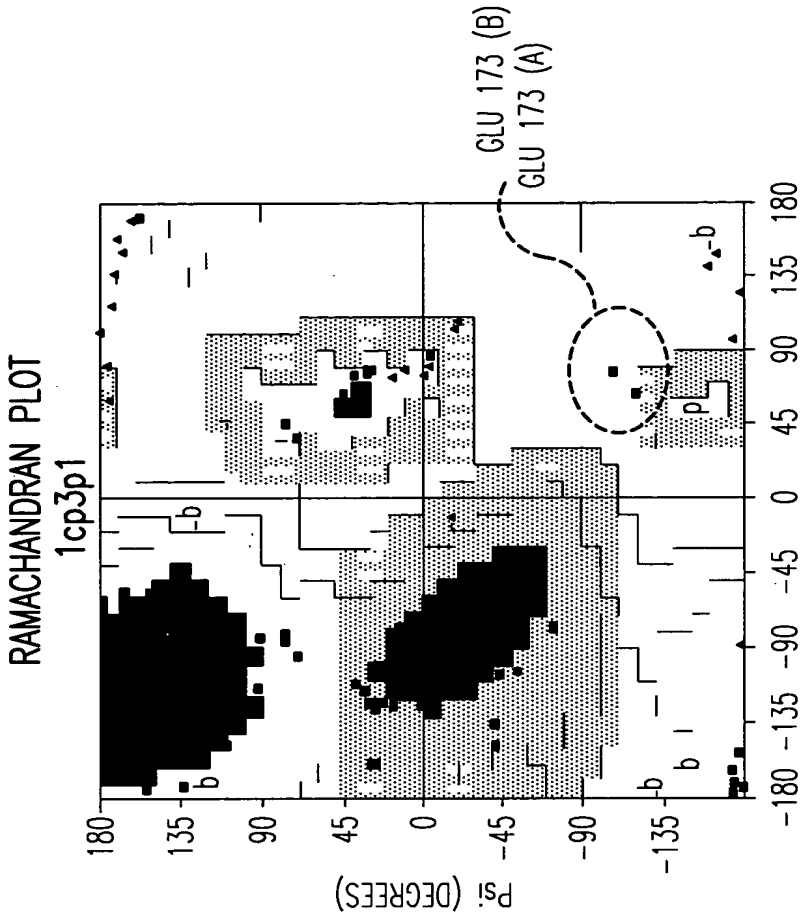

RAMACHANDRAN PLOT
1cp3p1
GLU 173 (B)
GLU 173 (A)
Psi (DEGREES)
PHi (DEGREES)
180
135
90
45
0
-45
-90
-135
-180

FIG.5B

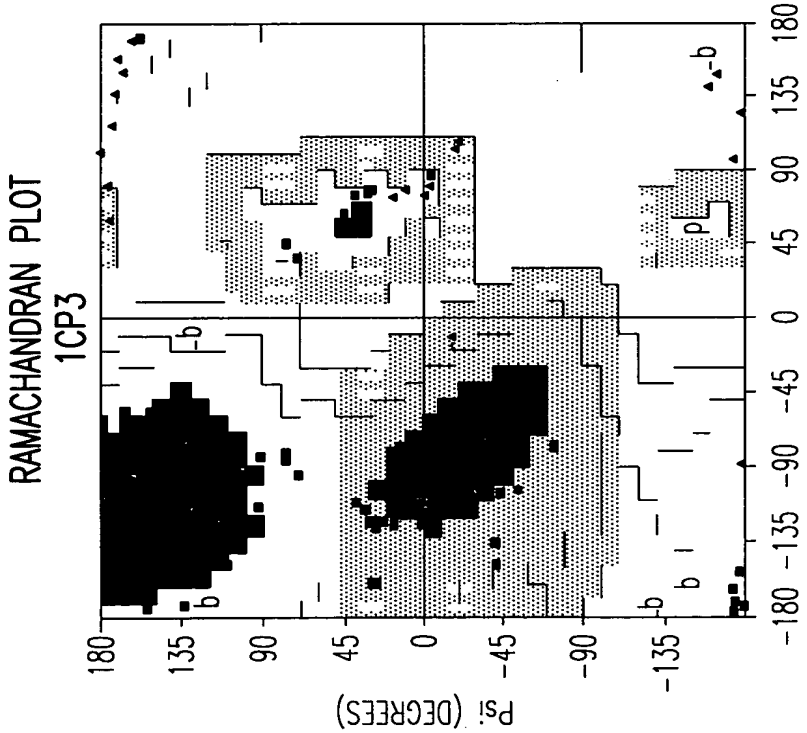

RAMACHANDRAN PLOT
1CP3
Psi (DEGREES)
PHi (DEGREES)
180
135
90
45
0
-45
-90
-135
-180

FIG.5A

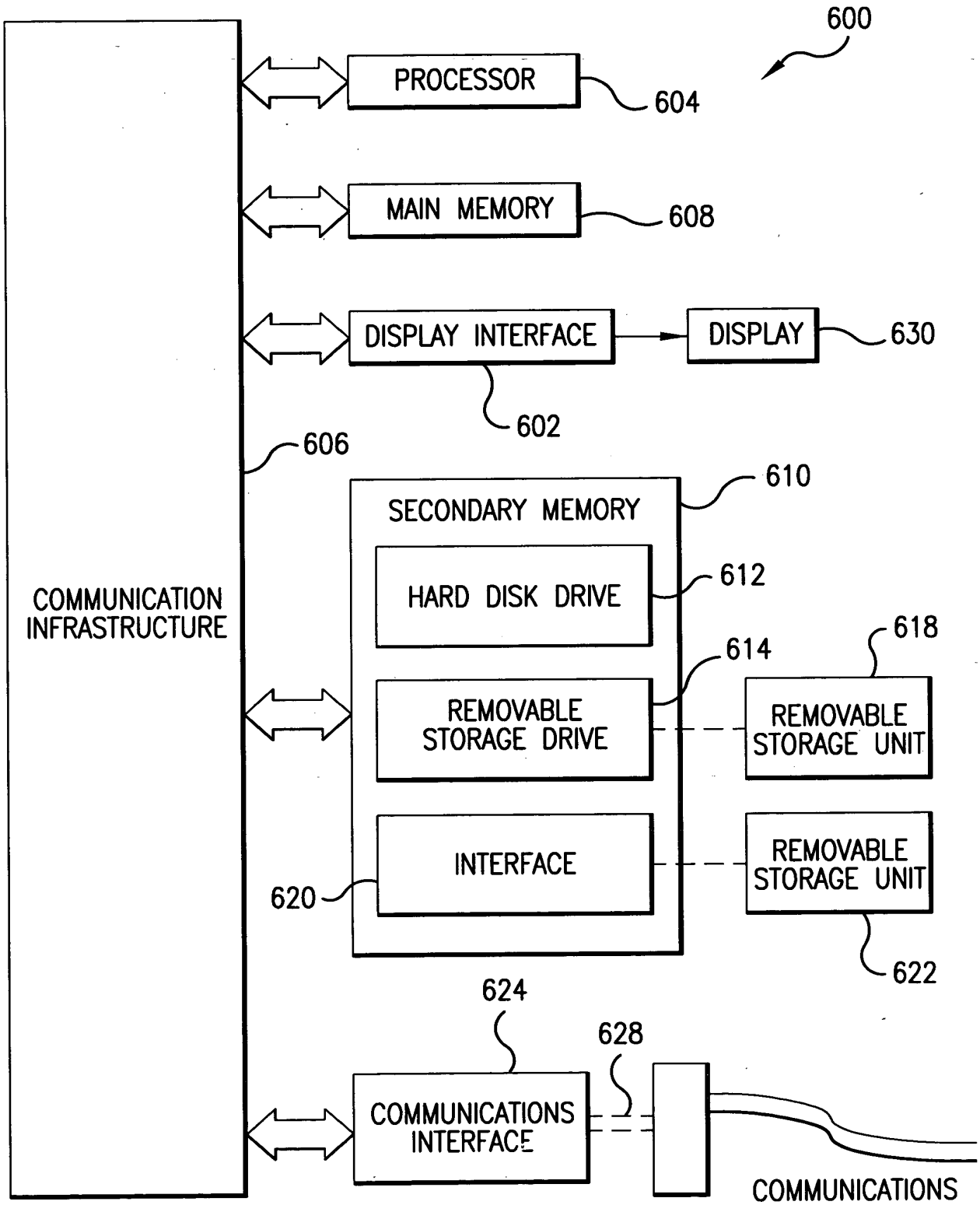

600
PROCESSOR
604
MAIN MEMORY
608
DISPLAY INTERFACE
DISPLAY
630
602
606
610
SECONDARY MEMORY
COMMUNICATION INFRASTRUCTURE
HARD DISK DRIVE
612
618
614
REMOVABLE STORAGE DRIVE
REMOVABLE STORAGE UNIT
INTERFACE
620
REMOVABLE STORAGE UNIT
622
624
628
COMMUNICATIONS INTERFACE
COMMUNICATIONS PATH
626

FIG.6

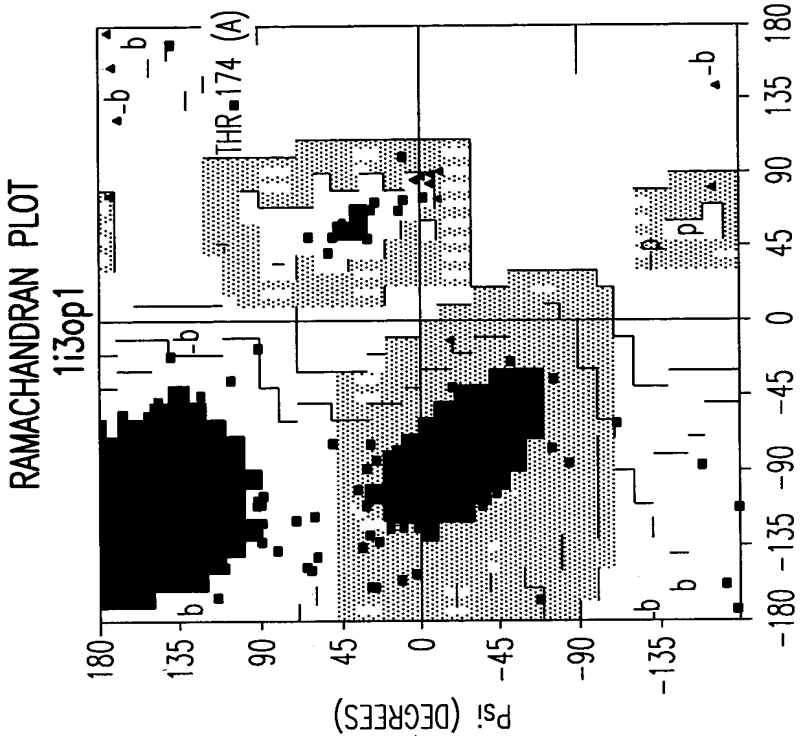

RAMACHANDRAN PLOT
1i3op1
THR-174 (A)
PSi (DEGREES)
PHi (DEGREES)
180
135
90
45
0
-45
-90
-135
-180
A
b
p

FIG.7B

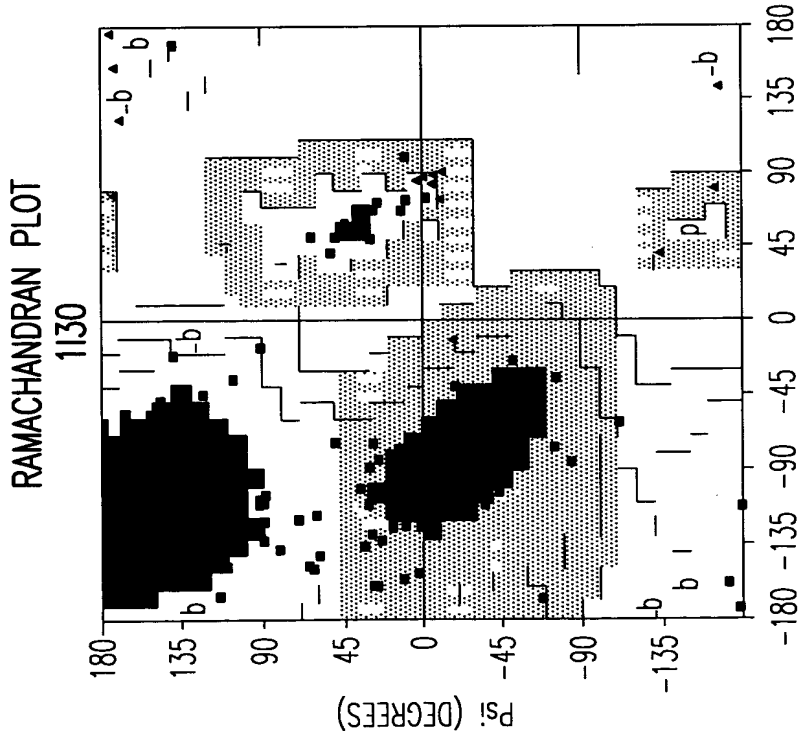

RAMACHANDRAN PLOT
1130
PSi (DEGREES)
PHi (DEGREES)
180
135
90
45
0
-45
-90
-135
-180
A
b
p

FIG.7A

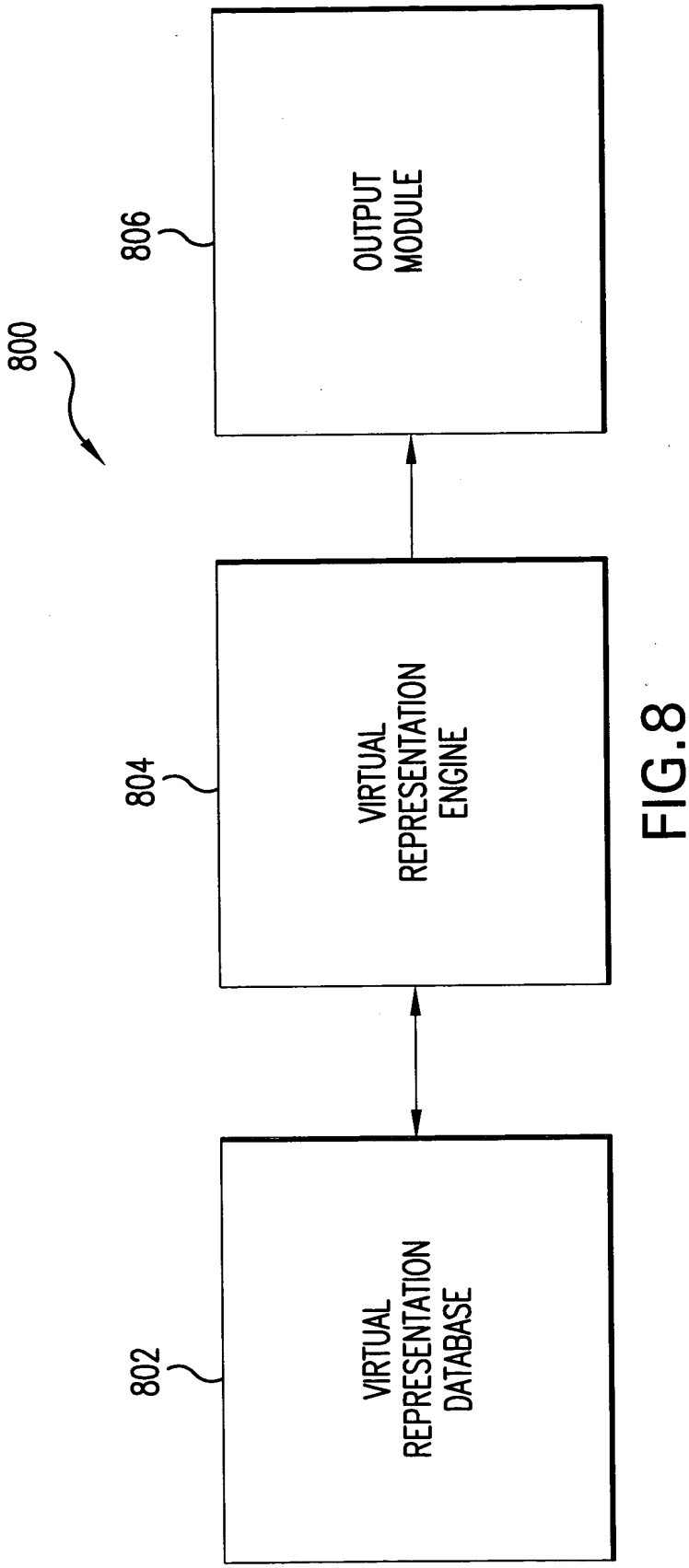
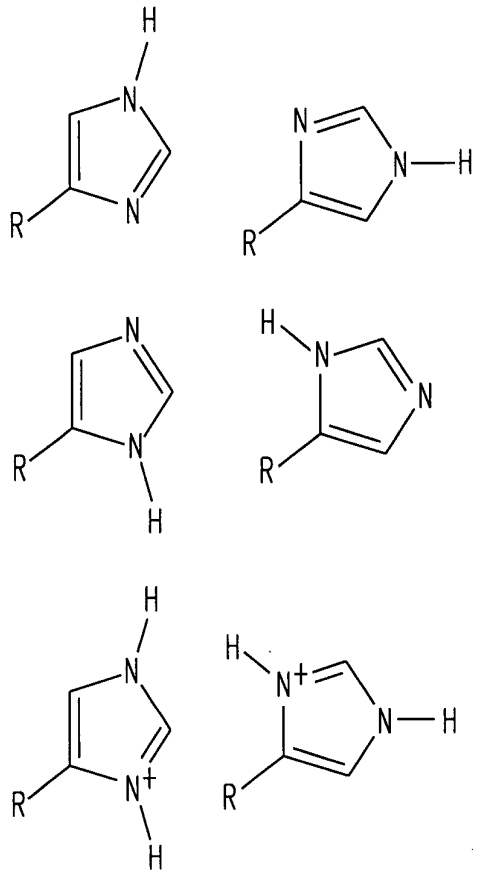
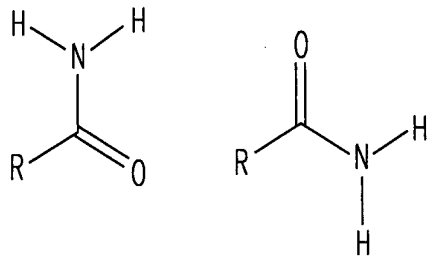

800
806
OUTPUT MODULE
804
VIRTUAL REPRESENTATION ENGINE
802
VIRTUAL REPRESENTATION DATABASE

FIG. 8

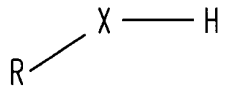
HISTIDINE TERMINI
(4 NEUTRAL CONFORMERS, 2 PROTONATED CONFORMERS, AS APPROPRIATE)



ASPARAGINE & GLUTAMINE RESIDUE TERMINI
(TWO CONFORMATIONS AS SHOWN BELOW)



TYROSINE, SERINE, CYSTEINE, THREONINE TERMINI
(MULTIPLE ROTOR STATES AROUND THE R–X BOND)



X=O,S

THE R IN EACH CASE IS THE REMAINDER OF SPECIFIC RESIDUE UNDER STUDY.

FIG.9

Sheet 22 of 22
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Title: Methods and Systems for Preparing Virtual Representations of Molecules